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(GOMD-S1-021-2018) A New Transferable Inter-Atomic Potential for Borosilicate Glasses

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Molecular dynamics simulations of borosilicate glasses are notoriously challenging due to various coordination states exhibited by boron atoms, which can be 3- or 4-fold coordinated. Here, we present a new empirical force-field for modified borosilicate glasses. Although the potential retains a simple formulation (2-body interactions, fixed partial charges, constant parameters), it is found to offer an excellent transferability to a wide range of compositions, from silicate to borate glasses. The evolution of the coordination number of boron atoms upon varying glass compositions is well reproduced.